



Substance

Beilstein Registry Number	3153371
Beilstein Preferred RN	95952-01-5
CAS Registry Number	95952-01-5
Chemical Name	palmitic acid <i>trans</i> -cinnamyl ester
Autoname	hexadecanoic acid 3-phenyl-allyl ester
Molecular Formula	C ₂₅ H ₄₀ O ₂
Molecular Weight	372.59
Lawson Number	5350, 1241
Structure Keyword	Stereo compound
Compound Type	isocyclic
Constitution ID	2352310
Tautomer ID	3027469
Beilstein Reference	4-06-00-03802, 5-06
Entry Date	1990/02/15
Update Date	1993/10/27

Reaction 1 of 3

Reaction ID	<u>423548</u>
Reactant BRN	3153371 palmitic acid <i>trans</i> -cinnamyl ester
Product BRN	<u>3167799</u> palmitic acid-((2 <i>RS</i> ,3 <i>SR</i>)-2,3-dibromo-3-phenyl-propyl ester)
No. of Reaction Details	1
Reaction Classification	Preparation
Reagent	CHCl ₃ bromine

Note 1	Handbook
Ref. 1	<u>1623868</u> ; Journal; Gonella; Abbattista; GCITA9; Gazz.Chim.Ital.; 85; 1955; 561, 565;

Reaction 2 of 3

Reaction ID	<u>1081208</u>
Reactant BRN	<u>741973</u> 3 <i>t</i> -phenyl-prop-2-en-1-ol <u>209105</u> 1-hexadecanoyl-1 <i>H</i> -imidazole
Product BRN	3153371 palmitic acid <i>trans</i> -cinnamyl ester
No. of Reaction Details	1
Reaction Classification	Preparation
Other Conditions	(i) imidazole, Na, THF, (ii) /BRN= 209105/
Note 1	Multistep reaction
Ref. 1	<u>36865</u> ; Journal; Staab,H.A.; Mannschreck,A.; CHBEAM; Chem.Ber.; GE; 95; 1962; 1284-1297;

Reaction 3 of 3

Reaction ID	<u>8078401</u>
Product BRN	3153371 palmitic acid <i>trans</i> -cinnamyl ester
No. of Reaction Details	1
Reaction Classification	Preparation (half reaction)
Other Conditions	(see original literature)
Note 1	Handbook
Ref. 1	<u>1623868</u> ; Journal; Gonella; Abbattista; GCITA9; Gazz.Chim.Ital.; 85; 1955; 561, 565;

Melting Point 1-2 of 2

VALUE (MP) C	Solvent (.SOL)	Note	Ref.
47	ethanol	1	1
46 - 46.5	ethanol		2

Note 1	Handbook
Ref. 1	<u>1623868</u> ; Journal; Gonella; Abbattista; GCITA9; Gazz.Chim.Ital.; 85; 1955; 561, 565;
Ref. 2	<u>36865</u> ; Journal; Staab,H.A.; Mannschreck,A.; CHBEAM; Chem.Ber.; GE; 95; 1962; 1284-1297;

Ultraviolet Spectra

Description		Spectrum
Solvent		ethanol
Note 1	220 - 295 nm	
Note 2	Handbook	
Ref. 1	<u>1623868</u> ; Journal; Gonella; Abbattista; GCITA9; Gazz.Chim.Ital.; 85; 1955; 561, 565;	

